

# Stabilization of the surface CDW order parameter by long-range Coulomb interaction

P. P. Aseev and S. N. Artemenko\*

*Institute for Radio-engineering and Electronics of Russian Academy of Sciences*

*Mokhovaya 11-7, Moscow 125009, Russia and*

*Moscow Institute for Physics and Technology*

*Institutski per. 9, Dolgoprudny, Russia*

(Dated: October 18, 2011)

## Abstract

We study theoretically formation of two-dimensional (2D) charge density wave (CDW) in a system of conducting chains at the surface of an insulator due to interaction of quasi 1D surface electrons with phonons. We show that the unscreened long-range Coulomb interaction between the charges induced by fluctuations of the CDW phase stabilizes the finite order parameter value at finite temperatures, and thus the long-range order (LRO) exists. In the case of screened Coulomb interaction the phase fluctuations suppress the phase transition, but decay of the order parameter is rather slow, it obeys a power-law  $\langle \Delta^*(r)\Delta(0) \rangle \propto r^{-\gamma}$  with small exponent  $\gamma$ .

PACS numbers: 71.45.Lr, 72.15.Nj, 73.20.Mf

In contrast to three-dimensional (3D) systems where fluctuations are usually small, in 2D systems fluctuations can greatly affect behaviour of a system. It is well-known<sup>1</sup> that in low-dimensional (1D and 2D) continuous systems with sufficiently short-range interaction a long-range order (LRO) is suppressed by long-range fluctuations. These fluctuations can be excited with little energy cost and they are favored since they increase the entropy. Thus, the 2D charge-density wave (CDW) phase is also believed to be suppressed by fluctuations of the CDW phase. However, there are experimental evidences of existence of 2D CDW in layered<sup>2</sup> and linear-chain compounds<sup>3</sup>. In the latter case it was shown that the critical temperature for a surface CDW in  $NbSe_3$  is higher than for a bulk one.

In a 2D superconductor which is related system, it is known<sup>4</sup> that there is no LRO indeed. Below the Berezinski-Kosterlitz-Thouless critical temperature, the correlation function of the order parameter obeys a power-law resulting in a pseudo-LRO in the system.

In this paper we examine the decay of the order parameter of the incommensurate CDW at the surface (commensurability is expected to stabilize the LRO).

The Mermin-Wagner theorem is applied<sup>1</sup> to the case of sufficiently short-range interaction. One of our goals is to study how the long-range Coulomb interaction may affect the LRO of the CDW. We consider three models of electron-electron interaction: non-screened Coulomb interaction, an interaction between surface electrons screened by electrons in the bulk, and an interaction between surface electrons screened only by surface electrons. The first case can be applied when the size of a sample is not greater than the screening radius. The second case refers to the systems where the bulk material is a semiconductor and there are electrons in the bulk or to systems with a gate. Finally, the third case refers to the systems in which the bulk material is an insulator and the only screening electrons are the electrons thermally excited over the Peierls gap of the 2D CDW.

Below we set  $\hbar$  and  $k_B$  to unity, restoring dimensional units in final expressions when necessary.

We study a system of conducting chains at the surface of a 3D insulator, electron system at the surface being considered as a 2D electron gas interacting with acoustic phonons in the bulk. We assume that  $x$ -axis is taken along the nesting vector  $Q$ .  $y$ -axis is taken perpendicular to the nesting vector and parallel to the surface. Finally,  $z$ -axis is the axis normal to the surface.

First, we consider the case of non-interacting electrons. The total action  $S$  is the sum of an action of free 2D electrons  $S_e$ , action of free phonons in the bulk  $S_{ph}$ , and action of electron-phonon interaction  $S_{e-ph}$

$$S = S_e + S_{ph} + S_{e-ph} \quad (1)$$

Only the phonons with the wave vector component along the surface (longitudinal component) close to the nesting vector  $\pm Q$  are relevant for formation of the CDW. If one does not take into account fluctuations of phonon modes one should consider only the modes with longitudinal component of wave vector equal to  $\pm Q$  exactly and the corresponding creation-annihilation operators  $\hat{b}_{\pm Q}$ ,  $\hat{b}_{\pm Q}^\dagger$ . However, since we take into account the fluctuations we allow the phonons to have the longitudinal component of the wave vector that slightly differs from  $Q$ . We describe these phonons with components of wave-vector  $\pm Q + q_x$ ,  $q_y$  and  $q_z$  (where  $q_x \ll Q$ ) using creation-annihilation operators  $\hat{b}_{\pm Q}(q_x, q_y, q_z)$ . The phonon field  $\hat{\varphi}$  is introduced in a standard way

$$\hat{\varphi}_Q(q, \omega) = \sqrt{\frac{\omega_0(q)}{2}} \left( \hat{b}_Q(q, \omega) + \hat{b}_{-Q}^\dagger(-q, -\omega) \right), \quad (2)$$

where  $\omega_0(q) = s\sqrt{(Q + q_x)^2 + q_y^2 + q_z^2}$  is the spectrum of acoustic phonons. Then the Matsubara action of free phonons reads

$$S_{\text{ph}} = -T \sum_{\omega} \int \frac{d^3q}{(2\pi)^3} \frac{\omega^2 + \omega_0^2(q)}{\omega_0^2(q)} |\varphi_Q(q, \omega)|^2, \quad (3)$$

where  $T$  is temperature, and  $q$  stands for all the three components  $q_x, q_y, q_z$

Since electrons are confined in the direction normal to the surface the electron field operator can be written as

$$\hat{\Psi}(x, y, z) = \hat{\Psi}(x, y)w(z)$$

where  $w(z)$  is the wave function of the ground mode of size quantization,  $w(z)$  decays exponentially in the depth of the bulk material:

$$W(z) = |w(x, y, z)|^2 = \kappa e^{-\kappa z} \quad (4)$$

We do not take into account higher transversal modes because their contribution is exponentially small at low temperatures. Besides, the low-temperature behaviour of the system and particularly the properties of CDW are determined by the electrons with energy close to the Fermi energy, and, therefore, with momentum close to  $\pm Q/2$ . Thus we can represent the electron field as

$$\hat{\Psi}(x, y) = e^{iQx/2}\hat{\psi}_+(x, y) + e^{-iQx/2}\hat{\psi}_-(x, y),$$

where  $\hat{\psi}_{\pm}(x, y)$  vary smoothly in comparison with the correspondent exponential factor. The Matsubara action of free electrons reads

$$S_e = \int \frac{d^2k}{(2\pi)^2} d\tau \{ \psi_+^* [\partial_{\tau} - \varepsilon_+] \psi_+ + \psi_-^* [\partial_{\tau} - \varepsilon_-] \psi_- \}, \quad (5)$$

where  $\varepsilon_{\pm} = \varepsilon_0(k \pm Q/2)$  and  $\varepsilon_0(k)$  is a spectrum of free electrons.

The term describing the electron-phonon interaction reads

$$S_{e-\text{ph}} = - \int d^3r' d^3r d\tau \psi_+^*(r) \psi_-(r) \times \\ \times W(z) g(r - r') \varphi_Q(r') + c.c. \quad (6)$$

We assume that the Fourier transform of interaction potential  $g(k) = \int d^3r g(r) e^{-ikr}$  may depend on the momentum  $k$ . Although we do not specify the particular dependence, note that such a dependence appears if one considers an electron-phonon interaction in a system with anisotropy.

It is convenient to introduce the order parameter as follows:

$$\Delta(k_x, k_y) = \int \frac{dq_z}{2\pi} \varphi_{Q, q_z}(k_x, k_y) g_{q_z}(k_x, k_y) W_{q_z} \quad (7)$$

where  $W_{q_z}$  is the Fourier transform of the square of transversal wavefunction (4)  $W_{q_z} = \int dz W(z) e^{-iq_z z}$ . The electron-phonon contribution to action (6) can be rewritten in terms of  $\Delta$  in a quite simple form

$$S_{e-\text{ph}} = - \int d^2r d\tau \{ \psi_+^* \psi_- \Delta + \Delta^* \psi_-^* \psi_+ \} \quad (8)$$

If one does not take into account fluctuations of the phonon modes then  $\Delta$  does not depend on coordinates and can be taken real. In this case one can calculate electron Green functions in imaginary time

$$G_{\pm\pm} = \langle \psi_{\pm}^{\dagger} \psi_{\pm} \rangle = \int \mathcal{D}\psi_{+}^{*} \mathcal{D}\psi_{+} \mathcal{D}\psi_{-}^{*} \mathcal{D}\psi_{-} \psi_{\pm}^{*} \psi_{\pm} e^{-S_e - S_{e-ph}}$$

and obtain the following expressions

$$G_{+-}(\varepsilon, k) = G_{-+}(\varepsilon, k) = -\frac{\Delta}{\varepsilon^2 + \xi^2 + \Delta^2}$$

$$G_{++}(\varepsilon, k) = -G_{--}^{*} = -\frac{-i\varepsilon + \xi}{\varepsilon^2 + \xi^2 + \Delta^2}$$

where  $\xi = \frac{\varepsilon_{+}(k) - \varepsilon_{-}(k)}{2} \approx v_F k_x$ . These Green functions correspond to an electron spectrum with a gap  $\varepsilon = \sqrt{\xi^2 + |\Delta|^2}$ . This result is similar to 3D case<sup>5</sup>.

It is convenient to integrate out the phonon fields and thus to derive an effective action for  $\Delta$ . Using the definition for  $\Delta$  (7) we obtain

$$\int \mathcal{D}\varphi_Q^{*} \mathcal{D}\varphi_Q e^{-S_{ph}} = \int \mathcal{D}\varphi_Q^{*} \mathcal{D}\varphi_Q \mathcal{D}\Delta^{*} \mathcal{D}\Delta \mathcal{D}\beta^{*} \mathcal{D}\beta \times$$

$$\times \exp \left\{ -S_{ph} + \beta^{*}(k_x, k_y) [\Delta(k_x, k_y) - \int \varphi_{Q,q_z}^{*}(k_x, k_y) g_{q_z}^{*}(k_x, k_y) W_{q_z}^{*} \frac{dq_z}{2\pi}] + c.c. \right\}$$

where  $\beta(k_x, k_y)$ ,  $\beta^{*}(k_x, k_y)$  are Lagrange multipliers for  $\Delta^{*}$  and  $\Delta$ . Performing Gaussian integration over  $\varphi, \varphi^{*}, \beta, \beta^{*}$  we obtain an effective action for  $\Delta$

$$S_{\Delta} = -T \sum_{\omega} \int \frac{dk_x dk_y}{(2\pi)^2} |\Delta(\omega, k)|^2 / F(\omega, k) \quad (9)$$

$$F(\omega, k) = \int \frac{dq_z}{2\pi} \frac{\omega_0^2(k, q_z)}{\omega^2 + \omega_0^2(k, q_z)} |g_{q_z}^2(k_x, k_y)| |W_{q_z}^2| \quad (10)$$

We can expand  $F(\omega, k)$  at small  $\omega$  and  $k$

$$F(\omega, k) = \frac{g_0^2 \kappa}{2} \left[ 1 - \frac{\omega^2 + s'^2 k^2}{s^2(Q^2 - \kappa^2)} \right]$$

where  $g_0 = g(k=0)$ , and  $s'$  can be roughly estimated as

$$s'^2 \approx s^2 \frac{|g(Q) - g_0|}{g_0} \quad (11)$$

We consider the case when  $Q > \kappa$ . If  $Q < \kappa$  the formation of CDW due to interaction with the phonons in the bulk is impossible.

Now we can minimize the total action given by (1), (5), (8), (9) and thus find the classical solution for the order parameter  $\Delta$  (i.e. the solution that does not take into account fluctuations of phonon field and, therefore, fluctuations of the order parameter). The equation for the classical  $\Delta$  resembles the self-consistent condition for the gap in the BCS theory

$$1 = \lambda \int \frac{1}{\sqrt{\varepsilon^2 - |\Delta|^2}} \tanh \frac{\varepsilon}{2T} d\varepsilon,$$

where  $\lambda = \frac{g_0^2 \kappa}{4\pi v_F a_y}$ ,  $a_y$  is a lattice constant in the direction normal to the nesting vector. The cut-off parameter at high energies is of order of  $\varepsilon_F$  and thus the solution at  $T = 0$  is  $\Delta = \varepsilon_F e^{-\lambda}$ . The result is similar to the case of CDW in 3D. The main feature of 2D systems is that in constrast to 3D, fluctuations are important in 2D. The main contribution to the fluctuations of the order parameter is given by fluctuations of the phase  $\chi$  where  $\Delta = \Delta_0 e^{i\chi}$ . The amplitude of the order parameter determines the Peierls energy gap, and fluctuations of the amplitude are described by the mode with a gap in the spectrum, in contrast to the long wavelength fluctuations of the phase which are related to gapless modes, so that at  $q \rightarrow 0$  they do not affect the total energy. Thus at  $T \ll \Delta$  we can ignore amplitude fluctuations, and it is convenient to rewrite the total action in terms of  $\chi$ . Then the phonon action reads

$$S_\Delta = -T|\Delta_0|^2 \sum_\omega \int \frac{d^2 q}{(2\pi)^2} \frac{\chi(\omega, q) \chi(-\omega, -q)}{F^2(\omega, q)}$$

The total effective action is

$$S_{\text{eff}}[\chi^*, \chi] = S_\Delta - \ln \int \mathcal{D}\psi_+^* \mathcal{D}\psi_+ \mathcal{D}\psi_-^* \mathcal{D}\psi_- e^{-S_e - S_{e-\text{ph}}} \quad (12)$$

Expanding the exponent in powers of  $\chi$  and leaving the second order terms, we perform Gaussian integration over  $\psi_\pm^*$ ,  $\psi_\pm$ . After some algebra we obtain the following effective action

$$S_{\text{eff}} = T \sum_\omega \int \frac{d^2 k}{(2\pi)^2} \frac{2|\Delta|^2}{g_0^2 \kappa} \times \left\{ \left[ \frac{\lambda}{2} + \frac{\omega^2 + s'^2 |k|^2}{s^2 (Q^2 + \kappa^2)} + \frac{\lambda \omega^2 + v_F^2 k_x^2}{6 |\Delta|^2} \right] \chi(\varepsilon, k) \chi(\varepsilon, k) + \left[ -\frac{\lambda}{2} + \frac{\lambda \omega^2 + v_F^2 k_x^2}{12 |\Delta_0|^2} \right] \chi(\varepsilon, k) \chi(-\varepsilon, -k) \right\}$$

Green function for  $\chi$  can be easily calculated

$$\langle \chi(\omega, k) \chi(-\omega, -k) \rangle = \int \mathcal{D}\chi \chi^2(\omega, k) e^{-S[\chi]} \quad (13)$$

$$\langle \chi(\omega, k) \chi(\omega, k) \rangle = \frac{\pi \lambda v_x^2 / (8v_F)}{\omega^2 + v_x^2 k_x^2 + s'^2 k_y^2} \quad (14)$$

where  $v_x^2 \simeq v_F^2 \frac{s^2 (Q^2 - \kappa^2)}{|\Delta|^2}$  is a velocity of excitations along the  $x$ -axis. Note that it follows from (11) that the velocity of excitations  $s'$  along the  $y$ -axis is non-zero if we take into account a dispersion of electron-phonon interaction  $g(k)$ . However, one would obtain non-zero

velocity of excitations along the  $y$ -axis if one took into account non-ideal nesting conditions. Thus we can assume that in a real setup the value of  $s'$  is of order of sound velocity  $s$ . The correlation function for phase  $\chi$  can be calculated as

$$\begin{aligned}\langle \chi(r, t) \chi(r + \delta r, t) \rangle &= \\ &= \sum_{\omega} \int \frac{d^2 k}{(2\pi)^2} \langle \chi(\omega, k) \chi(-\omega, -k) \rangle e^{ik\delta r} = \\ &= \frac{\pi \lambda}{32 v_F} \int \frac{d^2 k}{(2\pi)^2} \frac{e^{ik\delta r}}{\sqrt{v_x^2 k_x^2 + s'^2 k_y^2}} \coth \frac{\sqrt{v_x^2 k_x^2 + s'^2 k_y^2}}{2T} \quad (15)\end{aligned}$$

If the temperature  $T = 0$  then the correlation function for phase is finite and therefore the LRO exists in the system. Otherwise, if the temperature  $T > 0$ , the integral in (15) diverges at small  $k$  when  $\delta r = 0$ . Thus there is no long-range order at finite temperatures. However, the correlation function for the order parameter  $\langle \Delta^*(r, t) \Delta(r + \delta r, t) = |\Delta_0|^2 e^{-\langle [\chi(\delta r, t) - \chi(0, t)] \chi(0, t) \rangle}$  obeys the power-law

$$\langle \Delta^*(0) \Delta(r) \rangle = |\Delta_0|^2 (rQ)^{-\gamma_0}, \gamma_0 = \frac{\lambda v_x T a_y}{8 v_F \hbar s'}$$

The exponent  $\gamma_0$  is of order of  $\frac{T}{\Theta}$ , where  $\Theta$  is the Debye temperature.

In the presence of Coulomb interaction there is an addition contribution to the total energy, and thus to the total action (1), due to an interaction of charges induced by phase fluctuations. Given the phase  $\chi$ , the electron density can be calculated as

$$\rho = \int \mathcal{D}\psi_+^* \mathcal{D}\psi_+ \mathcal{D}\psi_-^* \mathcal{D}\psi_- (\psi_+^* \psi_+ + \psi_-^* \psi_-) e^{-S}$$

Thus we obtain the electron density induced by phase fluctuations  $\delta\rho = -e\partial_x \chi / (\pi a_y)$ .

The corresponding term in the action responsible for Coulomb interaction is given by

$$S_C = \int d\tau d^2 r_1 d^2 r_2 \delta\rho(r_1) V(r_1 - r_2) \delta\rho(r_2)$$

We consider three different models for Coulomb potential  $V(r_1 - r_2)$ : non-screened Coloumb potential, Coloumb potential screened by free electrons in 3D material, and Coloumb potential screened by thermally excited electrons in 2D electron layer.

First we consider non-screened Coulomb potential  $V(r) = e^2/(\epsilon^* r)$ , where  $\epsilon^*$  is effective dielectric constant. If the surface is a boundary between two media with dielectric constants  $\epsilon_1$  and  $\epsilon_2$ , then  $\epsilon^* = (\epsilon_1 + \epsilon_2)/2$ . Calculating the Green function for  $\chi$  by using (13) we obtain

$$\langle \chi(\omega, q) \chi(-\omega, -q) \rangle = \frac{\lambda \pi v_x^2 / (8 v_F)}{\omega^2 + \frac{2\lambda e^2 v_x^2}{\epsilon^* a_y v_F} q_x + s'^2 q_y^2}$$

The singularity at low frequencies is now integrable if  $T > 0$  as well, so the mean square of fluctuations of phase  $\langle \chi(r, t) \chi(r, t) \rangle$  is finite and therefore the LRO exists in the system.

Consider Coulomb interaction screened by free electrons in 3D, for example by electrons in a gate or by conduction electrons in a semiconductor. The interaction is described by Yukawa

potential  $V(r) = \frac{e^2}{\epsilon^* r} e^{-r/r_D}$ , where  $r_D$  is a screening radius. The Fourier transformation of this potential reads

$$V(q) = \int d^2r V(r) e^{-iqr} = 2\pi e^2 / \left( \epsilon^* \sqrt{q^2 + r_D^{-2}} \right),$$

and the Green function for  $\chi$  calculated using (13) has the form

$$\begin{aligned} \langle \chi(\omega, q) \chi(-\omega, -q) \rangle &= \\ &= \frac{\lambda \pi v_x^2 / (8v_F)}{\omega^2 + v_x^2 \left( 1 + 12\lambda \frac{e^2}{\epsilon^* v_F} \frac{r_D}{a_y} \right) q_x^2 + s'^2 q_y^2} \end{aligned}$$

The integral over  $\omega$  and  $q$  diverges at  $T > 0$  as in the case when there is no inter-electronic interaction, thus there is no LRO. However, the correlation function for  $\Delta$  obeys a power-law with different exponent.

$$\begin{aligned} \langle \Delta^*(0) \Delta(r) \rangle &= \Delta_0 \left( \frac{r}{r_D} \right)^{-\gamma_3}, \\ \gamma_3 &= \gamma_0 \sqrt{\frac{12\epsilon^* \lambda \hbar v_F}{e^2}} \sqrt{\frac{a_y}{r_D}} \end{aligned}$$

The exponent  $\gamma_3 \ll \gamma_0$ , and although there is only a short-range order in the system, the correlations decay more slowly and the system behaves like it has a real LRO provided the screening radius is large enough.

Finally, we consider the Coulomb interaction screened only by electrons thermally excited over the Peierls gap in the conducting 2D layer of width  $a_z$ . The Fourier transformation of the potential is given by

$$V(q) = 2\pi e^2 / \left[ \epsilon^* (|q| + a_z/r_D^2) \right]$$

Density of screening electrons and, therefore, the screening radius  $r_D$  depends exponentially on temperature  $r_D^2 \propto n_e^{-1} \propto e^{\Delta/T}$ .

The Green function for  $\chi$  calculated using (13) reads

$$\begin{aligned} \langle \chi(\omega, q) \chi(-\omega, -q) \rangle &= \\ &= \frac{\lambda \pi v_x^2 / (8v_F)}{\omega^2 + v_x^2 \left( 1 + 12\lambda \frac{e^2}{\epsilon^* v_F} \frac{r_D^2}{a_y a_z} \right) q_x^2 + s'^2 q_y^2} \end{aligned}$$

The integral over  $\omega$  and  $q$  diverges at  $T > 0$  again, and the correlation function for  $\Delta$  obeys a power-law but with a smaller exponent

$$\begin{aligned} \langle \Delta^*(0) \Delta(r) \rangle &= \Delta_0 (r a_z / r_D^2)^{-\gamma_2}, \\ \gamma_2 &= \frac{\sqrt{\lambda}}{16\sqrt{3}} \frac{v_x}{s'} \frac{T a_y}{\hbar v_F} \sqrt{\frac{\epsilon^* \hbar v_F}{e^2}} \sqrt{\frac{a_y a_z}{r_D^2}} \end{aligned}$$

The exponent  $\gamma_2 \ll \gamma_3 \ll \gamma_0$  for similar values of screening radius, and the correlations decay at greater distance than in the case of 3D screening or non-interacting electrons. Strictly saying, there is no LRO in the system but due to the very slow power-law decay of correlations there is a pseudo-LRO.

The work was supported by Russian Foundation for Basic Research and Russian Ministry of Education and Science (grant No 16.513.11.306).

---

\* Electronic address: art@cplire.ru

<sup>1</sup> N. Mermin, H. Wagner, Phys. Rev. Lett. 22 (1966), 1133.

<sup>2</sup> M. Marynowski, W. Franzen, M. El-Batanouny, V. Staemmler, Phys. Rev. B. 60 (1999), 6053

<sup>3</sup> C. Brun, Z.-Z. Wang, P. Monceau, S. Brazovskii, Phys. Rev. Lett. 104 (2010), 256403

<sup>4</sup> A. Larkin, A. Varlamov, Theory of Fluctuations in Superconductors (Oxford University Press, 2005) pp. 335–341

<sup>5</sup> S.N. Artemenko, A.F. Volkov, in: Charge Density Waves in Solids, ed. L.P. Gor'kov, G. Grüner (Elsevier Sci. Publ., Amsterdam, 1989), pp. 365–402